

1-Nitrobutane

627-05-4 | DTXSID8020967

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 6.99e-02 mol/L

Global applicability domain: Inside

Local applicability domain index: 7.53e-01

Confidence level: 5.97e-01

Nearest Neighbors from the Training Set

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1-Nitrobutane

Measured: 4.46e-02

Predicted: 6.99e-02

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2-Nitropropane

Measured: 2.15e-01

Predicted: 2.16e-01

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1-Nitropropane

Measured: 1.68e-01

Predicted: 2.14e-01

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Nitroethane

Measured: 6.26e-01

Predicted: 4.35e-01

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Dimethylglyoxime

Measured: 5.17e-03

Predicted: 2.01e-02